The Dynamic Structure Factor of the 1D Bose Gas near the Tonks-Girardeau Limit

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While the 1D Bose gas appears to exhibit superfluid response under certain conditions, it fails the Landau criterion according to the elementary excitation spectrum calculated by Lieb. The apparent riddle is solved by calculating the dynamic structure factor of the Lieb-Liniger 1D Bose gas. A pseudopotential Hamiltonian in the fermionic representation is used to derive a Hartree-Fock operator, which turns out to be well-behaved and local. The Random-Phase approximation for the dynamic structure factor based on this derivation is calculated analytically and is expected to be valid at least up to first order in $1/\gamma$, where γ is the dimensionless interaction strength of the model. The dynamic structure factor in this approximation clearly indicates a crossover behavior from the non-superfluid Tonks to the superfluid weakly-interacting regime, which should be observable by Bragg scattering in current experiments.

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The emergence of superfluidity at low temperatures is one of the most dramatic manifestations of quantum many-body physics in nature. Although the gas of interacting Bosons in 1D is described by the exactly solvable Lieb-Liniger (LL) model [1, 2], the question of superfluidity is not readily answered from the exact solutions. The dimensionless interaction parameter $\gamma = g_{\rm B}m/(\hbar^2 n)$ [1] governs the crossover from the weakly-interacting quasi-condensate for $\gamma \ll 1$ to the strongly-interacting Tonks-Girardeau gas [3] at $\gamma = \infty$, where $g_{\rm B}$ is the coupling constant of the 1D Bose gas [4], n is the line density, and m is the particle mass. The Landau criterion of superfluidity [5] predicts a critical velocity $v_{\rm c}$ for the breakdown of dissipationless flow if no elementary excitations of momentum p are accessible with energy below $pv_{\rm c}$ to dissipate its energy. The excitation spectrum of the LL model [2] contains umklapp excitations at finite momentum $2\pi n$ and energies which tend to zero in a large system predicting a critical velocity of zero by the Landau criterion *for any value of* γ [see the lower thin (blue) line in Fig. 1]. On the other hand, Luttinger-liquid theory and instanton techniques [6, 7] predict superfluidity in the LL model for sufficiently small γ. A resolution of this apparent paradox lies in the probability of excitation by an infinitesimal external perturber which is given by the dynamic structure factor (DSF) $S(q, \omega)$, the Fourier transform of the time-dependent density-density correlation function. A suppression of transitions in the vicinity of the umklapp excitation was found in Refs. [8, 9, 10]. In this Letter, we report a calculation of the DSF, valid for large γ as shown in Fig. 1. We find that even at fairly large but finite γ the low energy umklapp excitations are indeed suppressed while higher-energy excitations are enhanced. This is to be contrasted with the Tonks-Girardeau gas at $\gamma = \infty$ where all excitations are equally well accessible and prevent superfluidity.

Experiments have recently made significant progress in confining Bose gases in 1D [11] probing the strongly-correlated Tonks-Girardeau regime by increasing interactions up to values of $\gamma \approx 5.5$ [12] and to effective values of $\gamma_{\rm eff} \approx 200$ in an optical lattice [13]. In a recent experiment [14], the zero momentum excitations of a 1D Bose gas in an optical lattice have been measured by Bragg scattering, a technique that could also be used to measure the DSF.

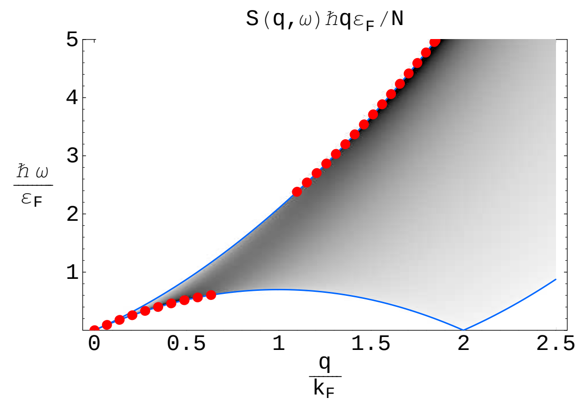

FIG. 1: Excitation spectrum at $\gamma = 13$. The upper and lower thin (blue) lines show the dispersions $\omega_+(q)$ and $\omega_-(q)$ of Eq. (14), respectively, limiting the elementary excitations of the LL model. The dynamic structure factor $S(q, \omega)$ in the approximation (8) is shown in shades of grey, between zero (white) and 1.0 $N/(\hbar q \varepsilon_{\rm F})$ (black). Here $k_{\rm F} = \pi n$ and $\varepsilon_{\rm F} = \hbar^2 k_{\rm F}^2/(2m)$. The the presence of a δ-function contribution is indicated by red dots.

Although the LL model is exactly solvable, it is notoriously difficult to calculate the various correlation functions. Many results in limiting cases are summarized in the book [15], but the full problem is not yet solved. Recently, progress has been made on various time-independent correlation functions [16, 17]. While a wealth of information is available for small γ where Bogoliubov's perturbation theory can be applied, the strongly-interacting regime was hardly accessible as a systematic expansion in γ^{-1} was lacking.

In this Letter we study the repulsively interacting 1D Bose gas in a fermionic representation, introduced as follows. The Bose-Fermi mapping of Girardeau [3] can be generalized [18] to map the 1D Bose gas with pair in-

teractions $V(x) = g_{\rm B}\delta(x)$ to an equivalent *interacting* Fermi system with the same excitation energies and the same absolute values of the associated wave functions. Hence, any observable has the same value in both representations if it derives from a local operator in coordinate space, *i.e.* is a function of the density operator $\hat{n}(x) = \sum_i \delta(x - x_i)$. In particular, this is the case for the DSF $S(q,\omega)$, which is the Fourier transform of the density-density correlation function [5, 19], and expresses the probability to excite a particular excited state through a density perturbation

$$S(q,\omega) = \sum_n |\langle 0|\hat{\rho}_q|n\rangle|^2 \delta(\hbar\omega - E_n + E_0), \tag{1}$$

where $\hat{\rho}_q = \sum_i \exp(-iqx_i)$ is the Fourier component of the density operator. In this mapping, large interactions between bosons correspond to small interactions between fermions, which allows for simple variational or perturbative treatment. However, the short-range interaction of Cheon and Shigehara [18] is highly singular for this purpose. It has been pointed out by Sen [20] that the ground state energy functional can be derived variationally with the pair-interaction pseudopotential

$$V_{\rm Sen}(x_1, x_2) = -g_{\rm F}\delta''(x_1 - x_2), \tag{2}$$

where $g_{\rm F} = 2\hbar^4/(m^2 g_{\rm B})$ is the coupling constant in the fermionic representation. This pseudopotential, however, is applicable only if the variational functions are continuous and vanish whenever two particle coordinates coincide. This is the case for Slater determinants which we will use later to derive the Hartree-Fock (HF) and Random-Phase approximations (RPA) but not for the exact fermionic wavefunctions [18]. $V_{\rm Sen}$ thus generates the first order correction to the ground-state energy easily whereas Sen found a renormalizable divergence in second order perturbation theory.

Recently, a more general pseudopotential was proposed by Girardeau and Olshanii [21], which is also defined for discontinuous functions and generates the correct energy functional for arbitrary values of the coupling constant. We give the following useful representation of this pseudopotential in terms of an integral kernel:

$$\begin{aligned} &V(x_1, x_2; x_1', x_2') = \\ &-2g_{\rm F}\delta\left(\frac{x_1 + x_2 - x_1' - x_2'}{2}\right)\delta'(x_1 - x_2)\delta'(x_1' - x_2'). \end{aligned} \tag{3}$$

Based on a pseudopotential Hamiltonian (2) or (3), we can derive the HF approximation and the generalized RPA giving access to the density-density correlation function and the static and dynamic structure factors. The results should be valid at least to first order in γ^{-1} and thus be useful near the Tonks-Girardeau limit of $\gamma = \infty$, where the interacting boson problem maps exactly to a free Fermi gas [3]. The purpose of this work is thus twofold: Besides predicting the behavior of correlation functions of the 1D Bose gas, we also test the validity and usefulness of the fermionic pseudopotential approach within the RPA.

The HF approximation for the fermionic system is derived variationally in the standard way. We find that both pseudopotentials (2) and (3) lead to exactly the same result: The HF equations for the single-particle orbitals $\varphi_j(x)$ take the usual form

$$\hat{F}\varphi_j(x) = \varepsilon_j \varphi_j(x). \tag{4}$$

Unlike the case of Coulomb interactions where the Fock operator $\hat{F}$ is nonlocal with a local Hartree and a nonlocal exchange term we find a purely local Fock operator

$$\begin{aligned} \hat{F} = &-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_{\rm ext}(x) \\ &+ g_{\rm F}\left[n(x)\frac{\partial^2}{\partial x^2} + 2\mathcal{P}(x)i\frac{\partial}{\partial x} - \mathcal{T}(x)\right]. \end{aligned} \tag{5}$$

The first two terms on the right hand side are just the single-particle part of the Hamiltonian. The mean-field parts in the square bracket involve the single-particle density $n(x) = \sum_j n_j \varphi^*{}_j(x)\varphi_j(x)$ and the derivative densities $\mathcal{P}(x) = -i\sum_j n_j \varphi^{*\prime}{}_j(x)\varphi_j(x)$ and $\mathcal{T}(x) = \sum_j n_j[\varphi_j^*(x)\varphi_j''(x) + 2\varphi^{*\prime}{}_j(x)\varphi_j'(x)]$, reminiscent of momentum and energy densities, respectively. Here, $\varphi' = {\rm d}\varphi/{\rm d}x$ and n_j is the fermionic occupation number $n_j = 1/\{\exp[(\varepsilon_j - \mu)/(k_{\rm B}T)] + 1\}$. At temperature $T = 0$, n_j defines the Fermi sea.

For the homogeneous gas ($V_{\rm ext} \equiv 0$), the quantum number j is associated with the particle momentum, and the single-particle orbital solutions of Eq. (4) are plane waves with energy and effective mass

$$\varepsilon_q = \hbar^2 q^2/(2m^*) - g_{\rm F}\pi^2 n^3/3, \tag{6}$$

$$m^* = m/\left(1 - 2g_{\rm F}mn/\hbar^2\right) = m/(1 - 4\gamma^{-1}), \tag{7}$$

respectively. The HF approximation for the ground-state energy coincides with the first two terms of the large-γ expansion of the exact ground-state energy in the LL model [1].

The HF approximation permits us to calculate the linear response function of time-dependent HF, also known as RPA with exchange or generalized RPA [19]. We calculate the DSF at zero temperature by the relation [19] $S(q,\omega) = {\rm Im}\{\chi(q, -\omega - i\varepsilon)/\pi\}$ for $\omega > 0$ and $S(q,\omega) = 0$ for $\omega < 0$ from the dynamic polarizability $\chi(q, \omega + i\varepsilon)$. The function $\chi(q, \omega + i\varepsilon)$ determines the linear density response to an external field [5, 19] and can be obtained from the linearized equation of motion of the density operator in the time-dependent HF approximation. In the Fourier representation of momentum and frequency, algebraic equations result which can be solved for $\chi(q,\omega)$. In the thermodynamic limit, the sums over momenta are replaced by integrals. We find $\chi(q,z) = \chi^{(0)}(q,z)/\{(1 - 4\gamma^{-1})[B - D\chi^{(0)}(q,z)]\}$, with

$z = \omega + i\varepsilon$ and $\varepsilon \to +0$. For the DSF this yields for $\omega > 0$

$$S(q,\omega) = \frac{-\chi_2^{(0)}(q,\omega) B}{\pi(1-4\gamma^{-1})\left[\left(B - D\chi_1^{(0)}\right)^2 + \left(D\chi_2^{(0)}\right)^2\right]} + \delta[\omega - \omega_0(q)] A(q), \quad (8)$$

where

$$B = 1 - 4\,(3\,\gamma - 16)/(\gamma - 4)^3, \quad (9)$$

$$D = \frac{4\varepsilon_{\rm F}}{N}\frac{\gamma}{(\gamma-4)^2}\left\{\frac{q^2}{k_{\rm F}^2}\frac{2\gamma - 9}{2\gamma} - \frac{2}{\gamma}\right. \quad (10)$$

$$\left. - \left[\frac{\hbar(\omega + i\varepsilon)\,k_{\rm F}}{\varepsilon_{\rm F} q}\right]^2 \frac{3\gamma - 16}{2(\gamma-4)^2}\right\}, \quad (11)$$

with the Tonks gas' Fermi wavenumber $k_{\rm F} = \pi n$ and energy $\varepsilon_{\rm F} = \hbar^2 k_{\rm F}^2/(2m)$. The polarizability $\chi^{(0)} = \chi_1^{(0)} + i\chi_2^{(0)}$ of the ideal 1D Fermi gas with renormalized mass. is given by the real and imaginary parts

$$\chi_1^{(0)}(q,\omega) = \frac{N m^*}{2\hbar^2 q k_{\rm F}} \ln\left|\frac{\omega^2 - \omega_-^2(q)}{\omega_+^2(q) - \omega^2}\right|, \quad (12)$$

$$\chi_2^{(0)}(q,\omega) = -\frac{N\pi m^*}{2\hbar^2 q k_{\rm F}}\begin{cases} \pm 1, & \omega_- \le \pm\omega \le \omega_+, \\ 0, & \text{else}, \end{cases} \quad (13)$$

where the dispersion relations

$$\omega_\pm(q) = \hbar|2k_{\rm F} q \pm q^2|/(2m^*) \quad (14)$$

border the continuum part of the accessible excitation spectrum made up from HF quasiparticle-quasihole excitations (6), see Fig. 1. The δ-function part of the DSF (8) relating to discrete excitations of collective character lies outside of the continuum part and comes from possible zeros in the denominator of $\chi(q,z)$. It is determined by the solution $\omega_0(q)$ of the transcendental equation $B - D\chi_1^{(0)} = 0$. We have solved this equation in various limits and found that at most one solution for $\omega_0(q)$ may exist. The strength $A(q)$ is given by the residue of χ at the pole $z = \omega_0(q) - i\varepsilon$. For small γ^{-1}, the strength $A(q) \simeq 2N\gamma \exp(-\gamma q/k_{\rm F})$ is exponentially suppressed and possible solutions are close to the dispersions $|\omega_0 - \omega_\pm| \propto \exp(-\gamma q/k_{\rm F})$. Due to this proximity of the discrete and continuous parts and expected smearing of discrete contributions beyond RPA, we may conjecture that the δ-function should be seen as part of the continuum, enhancing contributions near the border. In fact, we know from the exact solutions that energy spectrum is continuous [2].

At finite γ we find a δ-function contribution below and close to ω_- for small q whereas for large q there is a discrete contribution at energies larger than ω_+, see Fig. 1. In the limit $q \to \infty$ at finite γ, the δ part completely determines the DSF as the continuum part vanishes, and asymptotically $A \simeq N$, and $\omega_0 \simeq \hbar q^2/(2m)$ becomes the free particle dispersion reminiscent of the DSF for the weakly interacting Bose gas in Bogoliubov theory [5]. A more detailed analysis of the δ-function part will be given elsewhere [22].

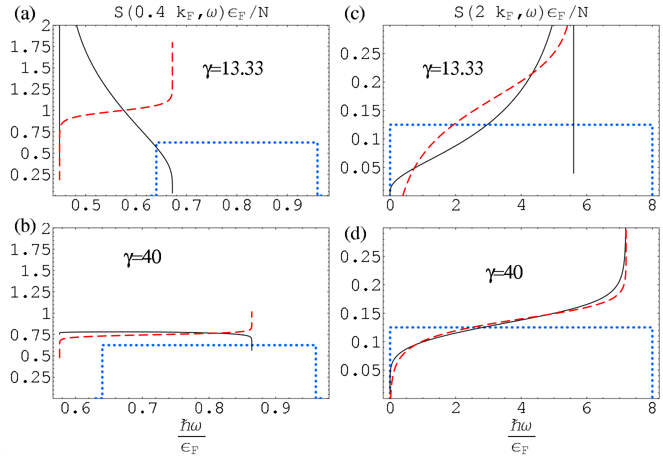

FIG. 2: DSF $S(q,\omega)$ as a function of ω at $q = 0.4k_{\rm F}$ [(a) and (b)] and $q = 2k_{\rm F}$ [(c) and (d)], and at interaction strength $\gamma = 13.33$ [(a) and (c)] and $\gamma = 40$ [(b) and (d)]. The solid (black) line shows the RPA result (8), the dashed (red) line shows the first order expansion in γ^{-1} (15), and the dotted (blue) line shows the DSF of the Tonks limit ($\gamma = \infty$) for comparison. While the first-order expansion always has a divergence to $+\infty$ near ω_+, the RPA result shows an enhancement of low-energy excitation near ω_- at small q. Note the unphysical negative values of the DSF in the first order expansion near ω_-, in particular for the umklapp excitations in panel (c).

The branches $\omega_\pm$ as shown in Fig. 1 are large γ approximations for the type I and II elementary excitation branches, respectively, introduced by Lieb [2]. In accordance with the exact results, both branches share the same slope at the origin and give rise to a single speed of sound given by $v_s \equiv {\rm d}\omega_\pm/{\rm d}k = \hbar k_{\rm F}/m^*$, which is the correct first order expansion of v_s for large γ [2]. Note that the usual Bogoliubov perturbation theory for weakly interacting Bosons gives a similar expansion of v_s for small γ and the type I excitation branch. Type II excitations are not described in the Bogoliubov theory.

Due to a logarithmic singularity in $\chi_1^{(0)}$, the DSF vanishes on the dispersion curves. For the Tonks gas at $\gamma \to \infty$, the value of the DSF within these limits is independent of ω and takes the value of $Nm/(2\pi\hbar^2 qn)$. The energy-dependence in the RPA for finite γ^{-1} is shown in Figs. 1 and 2. In particular, we see that the umklapp excitations at $q = 2k_{\rm F}$ at small ω, prohibiting superfluidity of the Tonks gas, are being suppressed. We find that $S(2k_{\rm F},\omega)$ in the RPA approaches zero as $1/\ln^2(\hbar\omega/\varepsilon_{\rm F})$, in contrast to the results [9, 10], predicting a power-law dependence on ω for finite γ based on a pseudoparticle-operator approach.

The RPA result may be expanded in $1/\gamma$, which yields

$$S(q,\omega)\frac{\varepsilon_{\rm F}}{N} = k_{\rm F}\frac{1 + 8\gamma^{-1}}{4q} + \frac{\ln f(q,\omega)}{2\gamma} + \mathcal{O}(\gamma^{-2}) \quad (15)$$

with $f(q,\omega) = |(\omega^2 - \omega_-^2)/(\omega_+^2 - \omega^2)|$. This expansion is supposed to be consistent with first order perturbation

theory. However, it can assume negative values as seen in Fig. 2 although $S(q,\omega)$ is known to be strictly non-negative, a property that is fulfilled by our RPA result (8). Close to ω_+, the first order expansion has has a logarithmic singularity to $+\infty$ which may be a precursor of the dominance of Bogoliubov-like excitations in the DSF at small γ. In the RPA this effect is even more pronounced due to a strong and narrow peak of the DSF in the RPA near ω_+ at large momenta as seen in Fig. 2. At finite gamma and for small momenta, however, the RPA predicts a peak near ω_-, contrary to the first-order result. Whether this effect is real or an artefact of the RPA is not obvious and may be decided by more accurate calculations or experiments. Spurious higher order terms in the RPA and an improved approximation scheme have been discussed in Ref. [23]. On the other hand, Roth and Burnett have recently observed a qualitatively similar effect in numerical calculations of the DSF of the Bose-Hubbard model [24].

We have verified numerically that the f-sum rule $m_1 \equiv \hbar^2 \int \omega S(q,\omega) \mathrm{d}\omega = N\hbar^2 q^2/(2m)$ is fulfilled, which should be an exact statement for the RPA from a general theorem [25]. The same follows also from the the large ω asymptotics of $\chi(q,\omega) \simeq 2m_1/(\hbar\omega)^2$ when χ is analytic as a function of ω in the upper half complex plane [5]. Our approximation breaks down when $\gamma \lesssim 8$ for small values of momenta $q \lesssim k_{\mathrm{F}}$, where imaginary poles of χ appear.

Our result (8) defines approximations for the static structure factor $S(q) = (\hbar/N)\int S(q,\omega)\mathrm{d}\omega$ and the pair correlation function $g(x) = 1 + \int [S(q) - 1]/(2\pi n)\exp(iqx)\mathrm{d}x$ that will be discussed in detail elsewhere [22]. Here we only note that the approximation for $S(q)$ is continuous and has the low-momentum expansion $S(q) = q[1+4\gamma^{-1} - q^2/(k_{\mathrm{F}}^2\gamma)]/(2k_{\mathrm{F}}) + \mathcal{O}(q^5)/\gamma + \mathcal{O}(\gamma^{-2})$. We also find that $g(x=0)$ vanishes in first order of γ^{-1} as consistent with Ref. [16], indicating once more the validity of our results.

Summarizing, we have derived variational approximations that should yield valid expansions of various correlation functions of the 1D Bose gas in $1/\gamma$, making predictions in a so-far unexplored regime. These approximations prove consistent with known limits and sum rules and therefore establish the usefulness of the fermionic pseudopotentials (2) and (3). We have also shown a rare example where a fully analytical calculation of the generalized RPA can be carried out for a non-trivial many-body system. Our results have immediate relevance to current experimental endeavors to explore fermionization in the strongly-interacting 1D Bose gas as they indicate qualitative deviation in the DSF from the Tonks gas limit already for very small γ^{-1}. The more accessible region of intermediate values of γ, which would yield more insight into the superfluid properties, is beyond the scope of this study. Answers may come from higher order or density-functional-theory based approximations extending the work of Ref. [26], from numerical calculations, or from experimental measurements. Obvious extensions of the present study to finite temperature, inhomogeneous systems, and periodic lattice potentials are under way.

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